L2 139 SEA SSS FUL L1

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=> s 12

L3 10 L2

=> d abs fbib hitstr 1-10

- L3 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN
- AB Theor. calcns. at semi-empirical AM1 and d. functional B3LYP/6-31G\* levels were carried out on 52 NH-indazoles. Although in most cases the 1H-tautomer is the most stable, we found several indazoles for which the 2H-tautomer is more stable than the 1H-tautomer. The differences in energy between the 1H- and 2H-tautomers were interpreted in terms of substituent effects with the use of a Free-Wilson (presence-absence) matrix.
- AN 2005:674931 CAPLUS
- DN 143:266493
- TI Theoretical estimation of the annular tautomerism of indazoles
- AU Alkorta, Ibon; Elguero, Jose
- CS Instituto de Quimica Medica, CSIC, Madrid, E-28006, Spain
- SO Journal of Physical Organic Chemistry (2005), 18(8), 719-724 CODEN: JPOCEE; ISSN: 0894-3230
- PB John Wiley & Sons Ltd.
- DT Journal
- LA English
- IT 42318-56-9, 1H-Pyrazolo[4,3-c]isoquinoline

RL: PRP (Properties)

(1H tautomer; theor. estimation of the annular tautomerism of indazoles)

- RN 42318-56-9 CAPLUS
- CN 1H-Pyrazolo[4,3-c]isoquinoline (9CI) (CA INDEX NAME)

RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN GI

Novel pyrazoloisoquinoline derivs. I, useful as kinase inhibitors, are AB disclosed [wherein: A = (un) substituted alkyl, OH or derivs., SH or derivs., CO2H or derivs., NH2 or derivs., cyano, (un) substituted heteroaryl, cycloalkyl, or heterocyclyl; B = bond, (un)substituted CH:CH, C.tplbond.C, O(CH2)1-4, O, S, CO, (un)substituted NH, NHCO, CONH, NHSO2, SO2NH, NHCONH, or C1-4 alkylene; D = (un) substituted alkyl, heteroaryl, heterocyclyl, aryl, or cycloalkyl; or BD = H, halo, fluoroalkoxy, (un) substituted alkyl; R = H, alkyl, (un) substituted arylalkyl; X, Z = H, alkyl, OH, alkoxy, halo, fluoroalkyl, CO2H or derivs., NH2 or derivs., cyano, SH or derivs., (un) substituted heterocyclyl or cycloalkyl; with provisos]. I are suitable for producing pharmaceuticals for the prophylaxis and therapy of diseases whose course involves an increased activity of NIK. Approx. 75 examples were prepared, and these plus addnl. compds. are individually claimed. For instance, 3-methoxybenzoic acid was condensed with 3-methyl-5-phenyl-1H-pyrazol-4-ylamine using HOBT and DIPC, and the resultant benzamide derivative was cyclized by treatment with P2O5 and POCl3 in xylene at 160°, to give title compound II. In a test for inhibition of release of IL1 $\beta$ , TNF $\alpha$ , and IL6 in LPS-stimulated heparinized whole human blood, II had IC50 values of 1.3, 1.2, and 7 μM, resp.

- AN 2005:120930 CAPLUS
- DN 142:219282
- TI Pyrazoloisoquinoline derivatives as kinase inhibitors, and their preparation, pharmaceutical compositions, and use in the treatment of diseases involving increased NIK activity.
- IN Majid, Tahir N.; Hopkins, Corey; Pedgrift, Brian L.; Collar, Nicola;
  Wirtz-Brugger, Friederike; Merrill, Jean
- PA Aventis Pharmaceuticals Inc., USA
- SO PCT Int. Appl., 94 pp.
- CODEN: PIXXD2
- DT Patent

LA English FAN.CNT 1

	PATENT NO.				KIN	D	DATE		APPLICATION NO.					DATE			
			<del>-</del>			_									-		
ΡI	WO 2005012301			A1 20050210		WO 2003-US21144					20030703						
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,
		PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	TJ,	TM,	TN,	TR,	TT,
		TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW					
	RW	: GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,
		KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,
		FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,
		BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG
									WO 2003-US21144				20030703				

OS MARPAT 142:219282

IT 112884-48-7P, 3-Methyl-5-phenyl-1H-pyrazolo[4,3-c]isoquinoline
645417-68-1P, 5-(3-Methoxyphenyl)-3-methyl-1H-pyrazolo[4,3c]isoquinoline 645417-70-5P, 5-(2-Methoxyphenyl)-3-methyl-1Hpyrazolo[4,3-c]isoquinoline 645417-71-6P, 5-(2,3Dimethoxyphenyl)-3-methyl-1H-pyrazolo[4,3-c]isoquinoline
645417-75-0P, 5-(3,5-Dimethoxyphenyl)-3-methyl-1H-pyrazolo[4,3c]isoquinoline 645417-93-2P, 5-Phenyl-1H-pyrazolo[4,3c]isoquinoline-3-carboxylic acid 645417-94-3P, Methyl
5-phenyl-1H-pyrazolo[4,3-c]isoquinoline-3-carboxylate
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)
 (drug candidate; preparation of pyrazoloisoquinoline derivs. as NIK inhibitors)

RN 112884-48-7 CAPLUS

CN 1H-Pyrazolo[4,3-c]isoquinoline, 3-methyl-5-phenyl- (9CI) (CA INDEX NAME)

RN 645417-68-1 CAPLUS

CN 1H-Pyrazolo[4,3-c]isoquinoline, 5-(3-methoxyphenyl)-3-methyl- (9CI) (CA INDEX NAME)

RN 645417-70-5 CAPLUS

RN 843613-16-1 CAPLUS

CN 1H-Pyrazolo[4,3-c]isoquinoline, 3-methyl-5-(naphthalenyl)-1-(phenylmethyl)(9CI) (CA INDEX NAME)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN GI

AB Title compds. [I; A = (substituted) alkyl, heteroaryl, heterocyclyl; B = bond, C:CR1, C.tplbond.C, O(CH2)a, O, S, CO, NR2, NR2CO, (substituted) alkylene, etc.; R1 = H, alkyl, aryl, etc.; R2 = alkyl, OH, alkoxy, halo, etc.; a = 1-4; D = (substituted) alkyl, heteroaryl, heterocyclyl, aryl, cycloalkyl; BD = H, halo, fluoroalkyl, fluoroalkoxy, etc.; R = H, alkyl, (substituted) aralkyl; X, Z = H, alkyl, OH, alkoxy, halo, fluoroalkyl, CO2R1, N(R1)2, cyano, SR1, SOR1, SO2R1, (substituted) heterocyclyl, cycloalkyl, etc.; with provisos], were prepared Thus, hydroxybenzotriazole, diisopropyl carbodiimide, benzoic acid, and 3,5-diphenyl-1H-pyrazol-4-ylamine were stirred 12 h in MeCN to give a residue which was heated with P2O5 and POCl3 in xylene at 150° for 4 h followed by stirring at room temperature for 12 h to give 3,5-diphenyl-1H-pyrazolo[4,3-c]isoquinoline. The latter inhibited TNFα release in LPS-stimulated human peripheral blood lymphocytes with IC50 = 1.9 nM.

AN 2005:34602 CAPLUS

DN 142:134600

TI Preparation of pyrazoloisoquinolines as NFkB-inducing kinase (NIK) inhibitors

IN Majid, Tahir Nadeem; Hopkins, Corey; Pedgrift, Brian Leslie; Collar,
Nicola; Wirtz-Brugger, Friederike; Merrill, Jean

PA Aventis Pharmaceuticals Inc., USA

SO U.S. Pat. Appl. Publ., 41 pp.

CODEN: USXXCO

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
ΡT	US 2005009859	 A1	20050113	US 2003-613588	20030703	
ΓI	05 2003009039	<b>7.</b>	20030113	US 2003-613588	20030703	

OS MARPAT 142:134600

IT 112884-48-7P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(claimed compound; preparation of pyrazoloisoquinolines as NFkB-inducing kinase inhibitors)

RN 112884-48-7 CAPLUS

CN 1H-Pyrazolo[4,3-c]isoquinoline, 3-methyl-5-phenyl- (9CI) (CA INDEX NAME)

IT112884-54-5P 112884-56-7P 824968-16-3P 824968-17-4P 824968-18-5P 824968-19-6P 824968-20-9P 824968-21-0P 824968-22-1P 824968-23-2P 824968-24-3P 824968-25-4P 824968-26-5P 824968-27-6P 824968-28-7P 824968-29-8P 824968-30-1P 824968-31-2P 824968-32-3P 824968-33-4P 824968-34-5P 824968-35-6P 824968-36-7P 824968-37-8P 824968-38-9P 824968-39-0P 824968-40-3P 824968-41-4P 824968-42-5P 824968-43-6P 824968-44-7P 824968-45-8P 824968-46-9P 824968-47-0P 824968-48-1P 824968-49-2P 824968-50-5P 824968-51-6P 824968-52-7P 824968-53-8P 824968-54-9P 824968-55-0P 824968-56-1P 824968-57-2P 824968-58-3P 824968-59-4P 824968-60-7P 824968-61-8P 824968-62-9P 824968-63-0P 824968-64-1P 824968-65-2P 824968-66-3P 824968-67-4P 824968-68-5P 824968-69-6P 824968-70-9P 824968-71-0P 824968-72-1P 824968-73-2P 824968-74-3P 824968-75-4P 824968-76-5P 824968-77-6P 824968-78-7P 824968-79-8P 824968-80-1P 824968-81-2P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (claimed compound; preparation of pyrazoloisoquinolines as NFkB-inducing kinase inhibitors)

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LA
     German
FAN.CNT 1
     PATENT NO.
                                             APPLICATION NO.
                                                                    DATE
                         KIND
                                 DATE
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     WO 2004005287
                                             WO 2003-EP6500
                                                                     20030620
PI
                          A1
                                 20040115
     WO 2004005287
                          C2
                                 20040304
             AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
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         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
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             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                           DE 2002-10229762
                                                                 A 20020703
     DE 10229762
                          A1
                                 20040122
                                             DE 2002-10229762
                                                                    20020703
     CA 2490571
                          AA
                                 20040115
                                             CA 2003-2490571
                                                                     20030620
                                             DE 2002-10229762
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                                             WO 2003-EP6500
                                                                 W
                                                                    20030620
     EP 1519934
                                             EP 2003-762498
                          A1
                                 20050406
                                                                     20030620
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
                                             DE 2002-10229762
                                                                 A 20020703
                                             WO 2003-EP6500
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     BR 2003012424
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                                 20050426
                                             BR 2003-12424
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                                             DE 2002-10229762
                                                                 A 20020703
                                             WO 2003-EP6500
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     US 2004097541
                          A1
                                 20040520
                                             US 2003-613482
                                                                     20030703
     US 6841556
                          B2
                                 20050111
                                             DE 2002-10229762
                                                                 A 20020703
                                             US 2002-423954P
                                                                    20021105
OS
     MARPAT 140:94041
IT
     645417-67-0P 645417-68-1P 645417-69-2P
     645417-70-5P 645417-71-6P 645417-72-7P
     645417-73-8P 645417-74-9P 645417-75-0P
     645417-76-1P 645417-77-2P 645417-78-3P
     645417-79-4P 645417-80-7P 645417-81-8P
     645417-82-9P 645417-83-0P 645417-84-1P
     645417-85-2P 645417-86-3P 645417-87-4P
     645417-88-5P 645417-89-6P 645417-90-9P
     645417-91-0P 645417-92-1P 645417-93-2P
     645417-94-3P 645417-95-4P 645417-96-5P
     645417-97-6P 645417-98-7P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (claimed compound; preparation of pyrazoloisoquinolines as NIK inhibitors)
     645417-67-0 CAPLUS
RN
     1H-Pyrazolo[4,3-c]isoquinoline, 3,5-diphenyl- (9CI) (CA INDEX NAME)
CN
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NAME)

RN 645417-97-6 CAPLUS

CN 1,3-Benzenediol, 5-(3-methyl-1H-pyrazolo[4,3-c]isoquinolin-5-yl)- (9CI) (CA INDEX NAME)

RN 645417-98-7 CAPLUS

CN 1,2-Benzenediol, 4-(3-methyl-1H-pyrazolo[4,3-c]isoquinolin-5-yl)- (9CI) (CA INDEX NAME)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

Addition-elimination reactions involving a nucleophile and a remote leaving group [SHN(AE)tele] are well-known under basic conditions, especially amongst electron-poor six-membered heterocycles, but are less commonly encountered for five-membered heterocycles and are rare under acidic conditions. Concentrated HCl converts 1-hydroxy-1H-pyrazolo[3,4-c] isoquinoline and 1-hydroxy-1H-pyrazolo[3,4-c]quinoline into 3-chloro-1H-pyrazolo[3,4-c]isoquinoline and 3-chloro-1H-pyrazolo[3,4-c]quinoline, resp. However, apparently neither the isomeric 1-hydroxy-1H-pyrazolo[4,3-c](iso)-quinolines nor the parent 1-hydroxypyrazole undergo this reaction. Addnl., all these systems are refractory under basic conditions. We present a plausible mechanism for the reaction, involving the 3-addition of Cl- to the diprotonated heterocycle, followed by the elimination of water.

Calcns. of the initial transition states and intermediates, using optimization at B3LYP/6-311+G(d,p), including thermochem. [HF/6-31+G(d)], and single-point Poisson-Boltzmann self-consistent reaction field determination of

the free energy of solvation (Jaguar Poisson-Boltzmann self-consistent reaction field), support this mechanism and reproduce the observed order of reactivity, the addition step being 2-4 kcal less favorable for the isomeric 1-hydroxy-1H-pyrazolo[4,3-c] (iso) quinolines and provide a rationalization for the role of strong acid.

AN 2003:353023 CAPLUS

DN 139:307390

TI Action of HCl on 3-hydroxypyrazolo(iso)quinolines to give 1-chloropyrazoles: evidence for an addition-elimination mechanism by ab initio calculations in gas phase and water

AU Greenwood, Jeremy R.; Begtrup, Mikael

CS Department of Medicinal Chemistry, Royal Danish School of Pharmacy, Copenhagen, Den.

Theoretical Chemistry Accounts (2003), 109(4), 200-205 CODEN: TCACFW; ISSN: 1432-881X

PB Springer-Verlag

DT Journal

LA English

IT 610272-18-9

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(ab initio study of reaction of hydrogen chloride with
3-hydroxypyrazolo(iso)quinolines to give 1-chloropyrazoles)

RN 610272-18-9 CAPLUS

CN 1H-Pyrazolo[4,3-c]isoquinoline, 1-hydroxy-, conjugate monoacid (9CI) (CA INDEX NAME)

#### ● H+

#### IT 610272-29-2

RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); FORM (Formation, nonpreparative); PROC (Process)

(ab initio study of reaction of hydrogen chloride with 3-hydroxypyrazolo(iso)quinolines to give 1-chloropyrazoles)

RN 610272-29-2 CAPLUS

CN 1H-Pyrazolo[4,3-c]isoquinoline, 3-chloro-, conjugate monoacid (9CI) (CA INDEX NAME)

• H+

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN GI

Ι

AB Regioselective bromination and iodination of pyrazoloquinolines and pyrazoloisoquinolines I and II (R = benzyl, R1 = H, X = N, Y = CH; R = benzyl, R1 = H, X = CH, Y = N) to form the corresponding halopyrazoles I and II (R1 = Br, I) was discussed. Reactivity differences between I (R = benzyl, R1 = H, X = N, Y = CH), I (R = benzyl, R1 = H, X = CH, Y = N) and II (R = benzyl, R1 = H, X = CH, Y = N), and the failure of II (R = benzyl, R1 = H, X = N, Y = CH) to give the expected halopyrazoles, were explained using calculated relative energies of bromination, and inspection of frontier MOs. Utility of the prepared halides was demonstrated by a series of palladium-catalyzed cross-coupling reactions.

II

AN 2001:246490 CAPLUS

DN 135:122430

TI Halogenation of pyrazoloquinolines and pyrazoloisoquinolines. Theoretical analysis of the regioreactivity and cross-coupling of 3-halogen derivatives

AU Pawlas, Jan; Greenwood, Jeremy; Vedso, Per; Liljefors, Tommy; Jakobsen, Palle; Huusfeldt, Per Olaf; Begtrup, Mikael

CS Department of Medicinal Chemistry, The Royal Danish School of Pharmacy, Copenhagen, DK-2100, Den.

SO Journal of the Chemical Society, Perkin Transactions 1 (2001), (8), 861-866

CODEN: JCSPCE; ISSN: 1472-7781

PB Royal Society of Chemistry

DT Journal

LA English

OS CASREACT 135:122430

# RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3ANSWER 7 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN 1-Hydroxypyrazolo[3,4-c]quinoline (I), 1-hydroxypyrazolo[4,3-c]quinoline  $\mathbf{AB}$ (II), 1-hydroxypyrazolo[3,4-c]isoquinoline (III), and 1hydroxypyrazolo[4,3-c]isoquinoline (IV) were prepared from 1-benzyloxypyrazole, establishing the pyridine B-ring in the terminal The pyridine ring of the 1-benzyloxy derivative of pyrazologuinolines II and I was formed via cyclization of a formyl group at C-4 or C-5 and an amino group of a 2-aminophenyl substituent at C-5 or C-4 in 1-benzyloxypyrazole. The pyridine ring of 1-benzyloxy derivs. of pyrazoloisoquinolines III and IV was created via cyclization of a formyl group in a 2-formylphenyl substituent at C-4 or C-5 with an iminophosphorane group installed at C-5 or C-4 of 1-benzyloxypyrazole by lithiation followed by reaction with tosyl azide and then with tributylphoshine utilizing the Staudinger/aza-Wittig protocol. 2-aminophenyl and the 2-formylphenyl substituent were introduced at C-5 or C-4 by regioselective metalation followed by transmetalation to the pyrazolylzinc halide and subsequent palladium-catalyzed cross-coupling with 2-iodoaniline or 2-bromobenzaldehyde. The order of reactions and use of protecting groups in the individual sequences have been optimized. 1-benzyloxy-substituted pyrazoloquinolines and isoquinolines thus obtained were debenzylated by strong acid to the corresponding 1-hydroxysubstituted pyrazoloquinolines and isoquinolines I-IV.

AN 2000:847300 CAPLUS

DN 134:147535

TI Synthesis of 1-hydroxy-substituted pyrazolo[3,4-c]- and pyrazolo[4,3-c]quinolines and -isoquinolines from 4- and 5-aryl-Substituted 1-benzyloxypyrazoles

AU Pawlas, Jan; Vedso, Per; Jakobsen, Palle; Huusfeldt, Per Olaf; Begtrup, Mikael

CS Department of Medicinal Chemistry, The Royal Danish School of Pharmacy, Copenhagen, DK-2100, Den.

SO Journal of Organic Chemistry (2000), 65(26), 9001-9006 CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

OS CASREACT 134:147535

IT 323582-69-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of hydroxy pyrazoloquinolines and -isoquinolines via cyclization of arylbenzyloxypyrazoles)

RN 323582-69-0 CAPLUS

CN 1H-Pyrazolo[4,3-c]isoquinoline, 1-(phenylmethoxy)- (9CI) (CA INDEX NAME)

IT 323583-17-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of hydroxy pyrazoloquinolines and -isoquinolines via cyclization of arylbenzyloxypyrazoles)

RN 323583-17-1 CAPLUS

CN 1H-Pyrazolo[4,3-c]isoquinoline, 1-hydroxy- (9CI) (CA INDEX NAME)

RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN GI

- \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT \*
- The tetrafluoroborate salts of triazoloquinolinium cation I, ABtriazolo[1,5-b]isoquinolinium cation II, and [1,2,3]triazolo[1,5a]pyrazinium cation III undergo valence bond isomerization when heated in either trifluoroacetic acid or in o-dichlorobenzene to ring-opened reactive intermediates which can participate in electrophilic substitution as nitrenium cations to yield pyrazole- and indazole-fused new heterocycles, pseudoelectrocyclization of nitrenium intermediates onto electron-deficient rings, or as carbenium cations in nucleophilic addition reactions. E.g., the tetrafluoroborate of II cyclized in o-dichlorobenzene at 190° to give the indazolylisoquinoline IV in 83% yield, while cyclization of II in CF3CO2H at reflux gave arylpyrazoloisoquinoline V in 85% yield. Comparison of these and some recent results reveals that this ring opening of fused [1,2,3]triazolium salts is a general phenomenon and is closely related to the well-known retro-electrocyclizations (called "1,5-dipolar cyclizations") of neutral fused [1,2,3] triazoles and tetrazoles.

AN 1999:392479 CAPLUS

DN 131:157733

TI Valence Bond Isomerization of Fused [1,2,3]Triazolium Salts with Bridgehead Nitrogen Atom. Fused Azolium Salts. 19

AU Beres, Mariann; Hajos, Gyoergy; Riedl, Zsuzsanna; Soos, Tibor; Timari,

Geza; Messmer, Andras

CS Chemical Research Center Institute of Chemistry, Hungarian Academy of Sciences, Budapest, H-1525, Hung.

SO Journal of Organic Chemistry (1999), 64(15), 5499-5503 CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

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LA English

OS CASREACT 131:157733

IT 237417-80-0P 237417-84-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of fused pyrazole and indazole heterocycles by valence bond isomerization ring cleavage and regioselective intramol. cyclization reactions of fused triazolium salts)

RN 237417-80-0 CAPLUS

CN 1H-Pyrazolo[4,3-c]isoquinoline, 1-(4-bromophenyl)-3-(4-chlorophenyl)(9CI) (CA INDEX NAME)

RN 237417-84-4 CAPLUS

CN 1H-Pyrazolo[4,3-c]isoquinoline, 1-(4-bromophenyl)-3-(2-thienyl)- (9CI) (CA INDEX NAME)

RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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